Triprolidine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 10.2

Global applicability domain: Inside

Local applicability domain index: 9.64e-01

Confidence level: 5.08e-01

Nearest Neighbors from the Training Set

Image not found
1,2,3,7,8-Pentachlorodibenzo-p-dioxin
Measured: 10.6
Predicted: 10.2

Image not found
cis-Chlordane
Measured: 8.90
Predicted: 9.58

Image not found
trans-Chlordane
Measured: 8.90
Predicted: 9.58

Image not found
2,3,4,7,8-Pentachlorodibenzofuran
Measured: 10.4
Predicted: 9.92

Image not found
1,2,3,8,9-Pentachlorodibenzofuran
Measured: 10.5
Predicted: 9.92

Image not found
1,2,3,4,7-Pentachlorodibenzo-p-dioxin
Measured: 10.7
Predicted: 9.59